Damage spreading in the mode-coupling equations for glasses

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We examine the problem of damage spreading in the off-equilibrium mode coupling equations. The study is done for the spherical p-spin model introduced by Crisanti, Horner and Sommers. For $p > 2$ we show the existence of a temperature transition T_0 well above any relevant thermodynamic transition temperature. Above T_0 the asymptotic damage decays to zero while below T_0 it decays to a finite value independent of the initial damage. This transition is stable in the presence of asymmetry in the interactions. We discuss the physical origin of this peculiar phase transition which occurs as a consequence of the non-linear coupling between the damage and the two-time correlation functions.

The theoretical understanding of the dynamical behavior of glasses is a long outstanding problem in statistical physics which has recently revealed new aspects related to the underlying mechanism responsible of the glass transition [1,2]. While there are still some obscure points in the theory (i.e. the inclusion of finite time activated process beyond the mean-field limit) a scenario has emerged which unifies the dynamical approach (mode-coupling theory) with the thermodynamic Adam-Gibbs-Di Marzio approach. The scenario for the dynamical behavior of glasses can be summarized in three different temperatures which separate three different regimes. In the high-temperature regime $T > T_d$ the system behaves as a liquid and is very well described by the mode-coupling equations of Götze in the equilibrium regime [3]. A crossover takes place at T_d where there is a dynamical singularity and the correlation functions do not decay to zero in the infinite time limit (ergodicity breaking). This dynamical singularity is a genuine mean-field effect which turns out to be a crossover temperature when activated processes are taken into account. Below T_d the relaxation time (or viscosity) starts to grow dramatically fast and seems to diverge at T_s where the configurational entropy vanishes and a thermodynamic phase transition takes place. The glass transition T_g (as defined where the viscosity is 10^{13} Poise) lies between T_s and T_d and depends on the cooling rate. Hence T_g does not correspond to a true dynamical singularity. Furthermore, there is a first order phase transition T_M where the liquid (if cooled sufficiently slow) crystallizes.

The essentials of this scenario have been corroborated in the context of mean-field spin glasses, and in particular in those models with a one step replica symmetry breaking transition [4]. While the first-order transition temperature T_M is absent in spin glasses (disorder prevents the existence of a crystal state) the other two transitions (T_s, T_d) have been clearly identified.

The purpose of this paper is the study of the damage spreading in models for structural glasses. Damage spreading is the study of the time propagation of a perturbation or damage in the initial condition of a system. The propagation of the initial damage is a dynamical effect which has deserved considerably attention in the past (specially in the context of dynamical systems, for instance, networks of boolean automata [5]) because it allows to explore the structure of the phase space of the system. To investigate damage spreading a suitable Hamming distance in the space of configurations is defined. Then we consider two random initial configurations $\{\sigma_i, \tau_i\}$ with a given initial distance D_0 for two identical systems which evolve under identical noise realizations and compute the distance $D(t)$ as a function of time. Eventually one is interested in the asymptotic long-time behavior of the distance $D(t)$, i.e $D_\infty = \lim_{t\to\infty} D(t)$. In general, three different regimes can be distinguished. A high-temperature regime $T > T_0$ where $D_\infty = 0$ independently of the initial distance D_0. A intermediate regime $T_1 < T < T_0$ where $D_\infty = D_\infty(T)$ is not zero but independent of the initial distance. And finally a low-temperature regime $T < T_1$ where $D_\infty = D_\infty(T, D_0)$ depends on both temperature and initial distance. While it is widely believed that T_1 corresponds to a thermodynamic phase transition it is not clear what the physical meaning of T_0 is.

In this work we address the problem of damage spreading in the off-equilibrium mode-coupling equations. We show the existence of the temperature T_0 in glasses well above T_d and T_s in the high temperature phase. We show that this new transition is a consequence of the non-linear coupling between the damage and the corresponding two-times correlation function. This effect is an essential ingredient of the mode-coupling equations and should be generally valid even beyond the mean-field limit. We believe the appearance of this damage transition is a quite general result in glassy models (with and without disorder) where the scenario of Götze for

mode-coupling transitions is valid.

The simplest solvable model which yields the off-equilibrium mode coupling equations is the spherical p-spin glass model [6]. In this case, the configurations are described by N continuous spin variables $\{\sigma_i; 1 \le i \le N\}$ which satisfy the spherical global constraint $\sum_{i=1}^N \sigma_i^2 = N$. The Langevin dynamics of the model is given by,

$$\frac{\partial \sigma_i}{\partial t} = F_i(\{\sigma\}) - \mu\sigma_i + \eta_i \tag{1}$$

where F_i is the force acting on the spin σ_i due to the interaction with the rest of the spins,

$$F_i = -\frac{\partial \mathcal{H}_i}{\partial \sigma_i} = \frac{1}{(p-1)!} \sum_{(i_2,i_3,\dots,i_p)} J_i^{i_2,i_3,..,i_p} \sigma_{i_2}\sigma_{i_3}..\sigma_{i_p} \tag{2}$$

and $\mathcal{H}$ is a Hamiltonian. The $J_i^{i_2,i_3,..,i_p}$ are quenched random variables with zero mean and variance $p!/(2N^{p-1})$ which we take to be symmetric under permutation of the different super indices. The calculations presented here can be easily generalized to asymmetric couplings [7]. Obviously, in this last case there is no energy $\mathcal{H}$ which drives the system to thermal equilibrium. The term μ in eq.(2) is a Lagrange multiplier which ensures that the spherical constraint is satisfied at all times and the noise η satisfies the fluctuation-dissipation relation $\langle \eta_i(t)\eta_j(s)\rangle = 2T\delta(t-s)\delta_{ij}$ where $\langle ... \rangle$ denotes the noise average.

We define the overlap between two configurations of the spins σ, τ by the relation $Q = \frac{1}{N}\sum_{i=1}^N \sigma_i\tau_i$ and the Hamming distance between these two configurations as,

$$D = \frac{1-Q}{2} \tag{3}$$

in such a way that identical configurations have zero distance and opposite configurations have maximal distance. Now we consider two copies of the system $\{\sigma_i, \tau_i\}$ which evolve under the same noise (1) but with different initial conditions. Here we restrict to random initial configurations (i.e equilibrium configurations at infinite temperature) with initial overlap $Q(0)$. Nevertheless, different type of initial conditions can be considered. The different set of correlation functions which describe the dynamics of the system are given by,

$$C(t,s) = \sum_{i=1}^N \sigma_i(t)\sigma_i(s) = \sum_{i=1}^N \tau_i(t)\tau_i(s) \tag{4}$$

$$R(t,s) = \sum_{i=1}^N \frac{\partial \sigma_i}{\partial h_i^\sigma} = \sum_{i=1}^N \frac{\partial \tau_i}{\partial h_i^\tau} \tag{5}$$

$$Q(t,s) = \sum_{i=1}^N \sigma_i(t)\tau_i(s) \tag{6}$$

where h_i^σ, h_i^τ are fields coupled to the spins σ_i, τ_i respectively. In what follows we take the convention $t > s$. The previous correlation functions satisfy the boundary conditions, $C(t,t) = 1, R(s,t) = 0, \lim_{t\to(s)^+} R(t,s) = 1$ while the two replica overlap $Q(t,s)$ defines the equal time overlap $Q_d(t) = Q(t,t)$ which yields the Hamming distance at equal times or damage $D(t)$ through the relation (3). Following standard functional methods [8,9] it is possible to write a closed set of equations for the previous correlation functions,

$$\frac{\partial C(t,s)}{\partial t} + \mu(t)C(t,s) = \frac{p}{2}\int_0^s du R(s,u)C^{p-1}(t,u) + \frac{p(p-1)}{2}\int_0^t du R(t,u)C(s,u)C^{p-2}(t,u) \tag{7}$$

$$\frac{\partial R(t,s)}{\partial t} + \mu(t)R(t,s) = \delta(t-s) + \frac{p(p-1)}{2}\int_s^t du R(t,u)R(u,s)C^{p-2}(t,u) \tag{8}$$

$$\frac{\partial Q(t,s)}{\partial t} + \mu(t)Q(t,s) = \frac{p}{2}\int_0^s du R(s,u)Q^{p-1}(t,u) + \frac{p(p-1)}{2}\int_0^t du R(t,u)Q(u,s)C^{p-2}(t,u) \tag{9}$$

while the Lagrange multiplier $\mu(t)$ and the diagonal correlation function $Q_d(t)$ obey the equations,

$$\mu(t) = T + \frac{p^2}{2}\int_0^t du R(t,u)C^{p-1}(t,u) \tag{10}$$

$$\frac{1}{2}\frac{\partial Q_d(t)}{\partial t} + \mu(t)Q_d(t) = T + \frac{p}{2}\int_0^t du R(t,u)Q^{p-1}(t,u) + \frac{p(p-1)}{2}\int_0^t du R(t,u)Q(t,u)C^{p-2}(t,u) \tag{11}$$

This set of equations is quite involved. For the correlation C and response functions R eqs.(7,8,10) several results are known, in particular their behavior in the FDT regime (where time translational invariance is satisfied and the fluctuation-dissipation theorem is obeyed) as well as in the aging regime [9].

A first glance to equations (9),(11) reveals that the overlap $Q(t,s)$ and its diagonal part $Q_d(t)$ are coupled each other through the correlation $C(t,s)$ and response function $R(t,s)$. The trivial solution $Q(t,s) = C(t,s)$ and $Q_d(t) = 1$ corresponds to the case where the initial conditions are the same, $Q_d(0) = 1$ and the distance $D(t) = 0$ for all times. This solution (hereafter we will denote it by HT) is asymptotically reached by the dynamics for high enough temperatures. The typical time needed to reach that solution grows if temperature decreases. At a given temperature (which we identify with T_0) there is an instability in the dynamical equations (9),(11) and the asymptotic solution differs from the HT one. We did not succeed in finding an explicit expression

for T_0 but we have been able to show its existence and find lower and upper bounds for its value.

To show the existence of T_0 we focus in the high temperature FDT regime $(t-s)/t << 1$ with t, s both large and $TR(t,s) = TR(t-s) = \frac{\partial C(t-s)}{\partial s}$. Writing $Q(t,s) = Q_d(s)\hat{Q}(t,s)$, using the inequalities $\hat{Q}(t,s) \leq C(t-s)$, $\frac{\partial Q_d(t)}{\partial t} \geq 0$ and inserting these results in (9) it is possible to get the following inequality,

$$T(1-Q_d(t)) + \frac{\beta Q_d(t)}{2}(Q_d^{p-2}(t)-1) \geq \frac{\partial Q_d(t)}{\partial t} \geq 0 \tag{12}$$

A trivial solution which always satisfies that inequality is $Q_d(t) = 1$. It is not difficult to check that the previous inequality yields a lower bound for the temperature at which there is an instability in the condition (12), leading to

$$T_0 \geq \sqrt{\frac{(p-2)}{2}} \quad . \tag{13}$$

On the other hand, a linear stability analysis of the equations (9),(11) around the HT solution, $Q_d(t) = 1 - \epsilon f(t)$, $Q(t,s) = C(t-s) - \epsilon g(t,s)$ where $f(0) = 1, g(t,t) = f(t)$ yields for equation (11) in the large t limit,

$$\frac{1}{2}\frac{\partial f}{\partial t} = -(T - \frac{p\beta}{2})f - \beta p \int_0^t du C^{p-1}(t-u)\frac{\partial g(t,u)}{\partial u} \quad . \tag{14}$$

Finally, the inequality $\frac{\partial g(t,u)}{\partial u} \geq 0$ together with (13) yields,

$$\sqrt{\frac{p}{2}-1} \leq T_0 \leq \sqrt{\frac{p}{2}} \tag{15}$$

As said before, it is very difficult to find an explicit expression for T_0. The reason is that both $Q_d(t)$ and $\hat{Q}(t,s)$ (or equivalently, $f(t)$ and $g(t,s)$ in the linear stability analysis) are not related by any FDT-like relation in the long time limit. Consequently, the analysis of the dynamic instability turns out to be more difficult.

Note that for the particular case $p = 2$ the inequality (15) yields $T_0 \leq 1$. Taking into account that (15) was derived under the assumption $T_0 \geq T_s = 1$ that yields $T_0 = 1$. The simpler case $p = 2$ has been already considered by Stariolo [10]

In the general case $p > 3$ a dynamical instability appears at temperatures well above any relevant thermodynamic temperature. In particular, for $p = 3$, numerical integration of the dynamical equations as well as the use of series expansions (see below) yields a dynamical transition at $T_0(p=3) = 1.04 \pm 02$ in agreement with the inequalities (15). Note that T_0 is much higher than $T_d(p=3) = 0.6125$ or $T_s(p=3) = 0.5$. The relaxation time τ_{relax} associated to the decay of the distance $D(t)$ to zero diverges according to a power law $\tau_{relax} \simeq (T-T_0)^{-\gamma}$ with $\gamma \simeq 1.1 \pm 0.1$.

It is important to note that T_0 is not related to any thermodynamic singularity. In the large p limit the inequality (15) yields $T_0 \to \sqrt{\frac{p}{2}}$ which gives a temperature much above the TAP temperature where an exponentially large number of states start to appear ($T_{TAP} \to \sqrt{\log(p)}$). Consequently, the origin of the damage spreading transition is purely dynamical and not related to any thermodynamic singularity or even to the existence of an exponentially large number of metastable states in the system.

Now we discuss the behavior of the asymptotic distance below T_0. In principle a new transition at T_d (which we identify as T_1) is expected for the dynamical behavior of $Q_d(t)$ because the correlation C develops the mode-coupling instability. We will see that for $p > 2$ the transition temperature T_1 is absent. It is very difficult to get analytical results below T_d. A possible way to investigate the asymptotic long-time limit of Q_d in the low-temperature regime (i.e below T_0) is to numerically integrate the set of dynamical equations (7)-(11). Unfortunately, the CPU time and the memory needed to numerically integrate them grows very fast with the maximum time t (approximately like t^2). On the other hand, $Q_d(t)$ displays in several cases a non monotonic behavior as a function of time. Consequently, it is very difficult to extrapolate the numerical data to the infinite time limit.

An alternative method was recently proposed in [11] were the series expansion for correlation and response functions was used to investigate the asymptotic long time limit of quantities such as the internal energy. Here we follow [11] but extend their method within the constrained formalism to include the series expansions for the correlation function $Q(t,s)$. To this end, we decompose in Taylor series the correlation, the response as well as the overlap,

$$C(t,s) = \sum_{k=0}^{\infty}\Big(\sum_{l=0}^{k} c_{kl}(t-s)^l t^{k-l}\Big) \tag{16}$$

$$R(t,s) = \sum_{k=0}^{\infty}\Big(\sum_{l=0}^{k} r_{kl}(t-s)^l t^{k-l}\Big) \tag{17}$$

$$Q(t,s) = \sum_{k=0}^{\infty}\Big(\sum_{l=0}^{k} q_{kl}(t-s)^l t^{k-l}\Big) \tag{18}$$

$$\mu(t) = \sum_{k=0}^{\infty} \mu_k t^k \tag{19}$$

where $c_{k0} = r_{k0} = \delta_{k0}$ and $Q_d(t) = \sum_{k=0}^{\infty} q_{k0} t^k$. It is possible to write in this case the recurrence relations between the different coefficients $c_{kl}, r_{kl}, q_{kl}, \mu_k$. The time necessary to calculate the first coefficients of the series is

not very large and takes a few hours in a work station to reach the first 80 terms of the series *. The radius of convergence of these series is quite small. To enlarge their radius of convergence we have used Pade approximants to get an estimate of the asymptotic value of the distance $Q_d(\infty)$. While the method works very well in case of the asymptotic value of the energy [11] (which depends on the Lagrange multiplier μ via the relation $\mu = T - pE(t)$) it is less effective for the asymptotic distance. The reason is that, while $\mu(t)$ is a monotonous increasing function of time, $Q_d(t)$ is not. In fact, below T_0 the overlap $Q_d(t)$ has a maximum as a function of time for some values of T and the initial condition $Q_d(0)$. Consequently, the complex function $Q_d(z)$ turns out to have zeros close to the real axis and the radius of convergence of the Pades is smaller. But still it is possible to obtain some estimates for the asymptotic distance. Numerical integrations of the dynamical equations have been used to check that our extrapolations in the infinite time limit are correct.

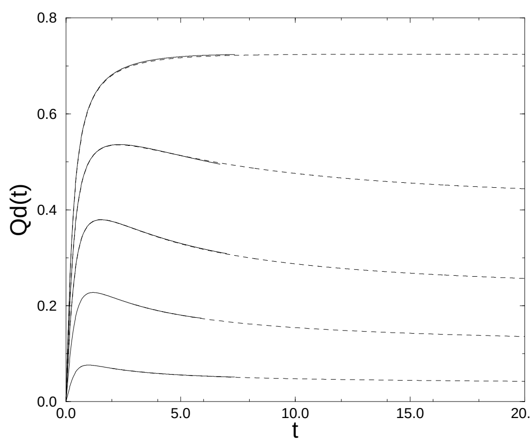

FIG. 1. $Q_d(t)$ with $Q_d(0) = 0$ as a function of time for different temperatures. From top to bottom $T = 0.9, 0.7, 0.5, 0.3, 0.1$. The continuous lines are the numerical integrations with time step $\Delta t = 0.01$ and the dashed lines are the reconstructed functions obtained from the Pade analysis.

Some of our results are shown in figures 1 and 2 for case $p = 3$. We have studied three different initial conditions: a) anti-correlated random initial conditions with $Q_d(0) = -1$, b) uncorrelated random initial conditions with $Q_d(0) = 0$ and c) partially correlated random initial conditions with $Q_d(0) = 0.5$. Case a) was analyzed using diagonal and the first off-diagonal Pade approximants assuming an asymptotic power law decay $Q_d(t) = Q_d(\infty) + At^{-\gamma}$. Cases b) and c) turned out to be more difficult to analyze due to the small radius of convergence of the series as well as to the presence of poles in the Pades.

The behavior of $Q_d(t)$ for case b) is shown in figure 1 for different temperatures. The continuous line corresponds to the numerical integration of the dynamical equations while the dashed lines are the reconstructed functions $Q_d(t)$ obtained from the Pade analysis. Note the presence of a maximum in $Q_d(t)$ for several different temperatures. This feature is a consequence of the non-linear character (in Q) of equations (9,11) for $p \geq 3$ and is absent for $p = 2$ [10].

Figure 2 shows the asymptotic distance D_∞ for cases a),b) and c) as a function of the temperature. We find that the asymptotic distance is independent of the initial correlation. This is an interesting result since one would expect (at least below T_d) a dependence on the initial condition. We have to note that the dependence on the initial conditions is expected for models with the symmetry $\sigma \to -\sigma$ and with a simple free energy landscape. If the initial distance D_0 is not zero there is always a finite probability (depending on D_0) that the initial configurations start in different (symmetry related) ergodic components. Consequently, the asymptotic distance depends on the initial value of D_0. Here, such behavior is only found for $p = 2$ [10].

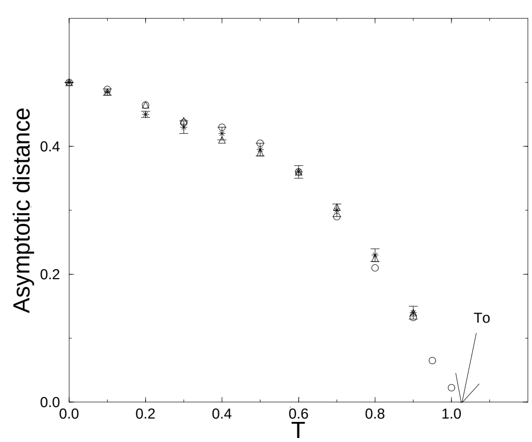

FIG. 2. Asymptotic distance D_∞ for $p = 3$ obtained from the Pade analysis of the series expansions for different initial conditions $D_0 = 1$ (circles), $D_0 = 0.5$ (triangles), $D_0 = 0.25$ (stars). Typical error bars are shown for the last case.

*This is true for case $p = 3$ while for larger values of p the computational effort is larger

In summary, we have studied the spreading of damage in the off-equilibrium mode-coupling equations. We have explicitly shown the existence of a damage spreading transition T_0 and also found lower and upper bounds for its value. This transition takes place at very high temperatures. On the other hand, this transition is completely unrelated to the existence of metastable states in the system. In fact, we have observed that this transition is quite stable to the inclusion of any degree of asymmetry. Indeed in the fully asymmetric case we find that $T_0 \simeq 0.71$ for $p = 3$. Consequently, the damage spreading transition persists in the absence of the spin-glass phase or even in the absence of metastable states. This result corroborates some results already found for other disordered spin-glass models [12,13]. Interestingly, equations (9,11) show that, only for $p > 2$, the coupling between the damage $Q_d(t)$ and the two-time correlation function $Q(t, s)$ is non linear. This non-linear coupling is crucial for the appearance of the damage transition T_0 which is well above T_d. We have also shown that below T_0 the asymptotic distance is independent of the initial distance. This was unexpected since such a dependence has been usually found in numerical investigations of several spin-glass models [14]. It would be interesting to understand whether this result is a direct consequence of the first order nature of the glass transition. This and other issues, such as the scaling behavior of the overlap $Q(t, s)$ in the aging regime and the existence of this transition in non-disordered glass forming liquids are left for future investigations.

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